

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.11e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.33e-01

Confidence level: 4.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Bromacil</div> <div>Measured: 3.12e-03</div> <div>Predicted: 3.11e-03</div>	<div>Image not found</div> <div>Isocil</div> <div>Measured: 8.70e-03</div> <div>Predicted: 5.23e-03</div>	<div>Image not found</div> <div>Terbacil</div> <div>Measured: 3.28e-03</div> <div>Predicted: 5.13e-03</div>
<div>Image not found</div> <div>Lenacil</div> <div>Measured: 2.56e-05</div> <div>Predicted: 1.78e-04</div>	<div>Image not found</div> <div>DKA 24</div> <div>Measured: 9.13e-02</div> <div>Predicted: 2.17e-02</div>	